Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 09:27 AM EDT

PDB ID	:	7L21
Title	:	Pyruvate Kinase M2 mutant-N70D
Authors	:	Nandi, S.; Dey, M.
Deposited on	:	2020-12-16
Resolution	:	2.29 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
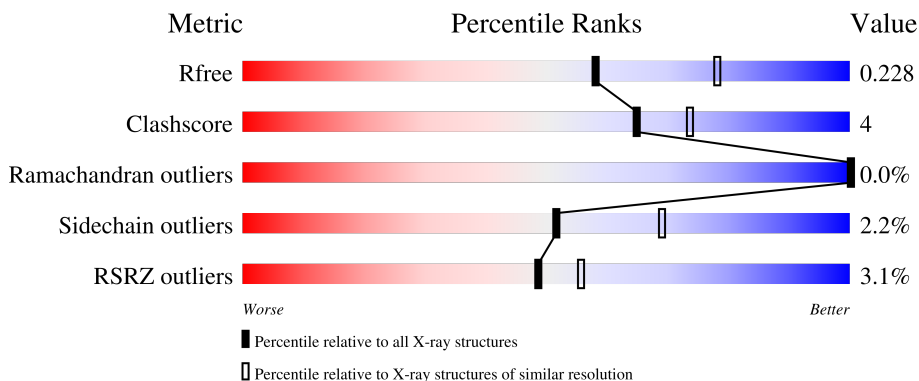
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	550	2% / 85% / 8% / 6%
1	B	550	.% / 83% / 10% / 6%
1	C	550	2% / 85% / 9% / 6%
1	D	550	7% / 79% / 12% / • / 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OXL	A	601	-	X	-	-
2	OXL	B	601	-	X	-	-
2	OXL	D	601	-	X	-	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 16070 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pyruvate kinase PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total 3878	C 2437	N 686	O 730	S 25	0	0	0
1	B	515	Total 3862	C 2430	N 677	O 730	S 25	0	0	0
1	C	518	Total 3886	C 2441	N 688	O 732	S 25	0	0	0
1	D	504	Total 3661	C 2291	N 659	O 688	S 23	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP P14618
A	-17	GLY	-	expression tag	UNP P14618
A	-16	SER	-	expression tag	UNP P14618
A	-15	SER	-	expression tag	UNP P14618
A	-14	HIS	-	expression tag	UNP P14618
A	-13	HIS	-	expression tag	UNP P14618
A	-12	HIS	-	expression tag	UNP P14618
A	-11	HIS	-	expression tag	UNP P14618
A	-10	HIS	-	expression tag	UNP P14618
A	-9	HIS	-	expression tag	UNP P14618
A	-8	SER	-	expression tag	UNP P14618
A	-7	SER	-	expression tag	UNP P14618
A	-6	GLY	-	expression tag	UNP P14618
A	-5	LEU	-	expression tag	UNP P14618
A	-4	VAL	-	expression tag	UNP P14618
A	-3	PRO	-	expression tag	UNP P14618
A	-2	ARG	-	expression tag	UNP P14618
A	-1	GLY	-	expression tag	UNP P14618
A	0	SER	-	expression tag	UNP P14618
A	70	ASP	ASN	engineered mutation	UNP P14618
B	-18	MET	-	initiating methionine	UNP P14618

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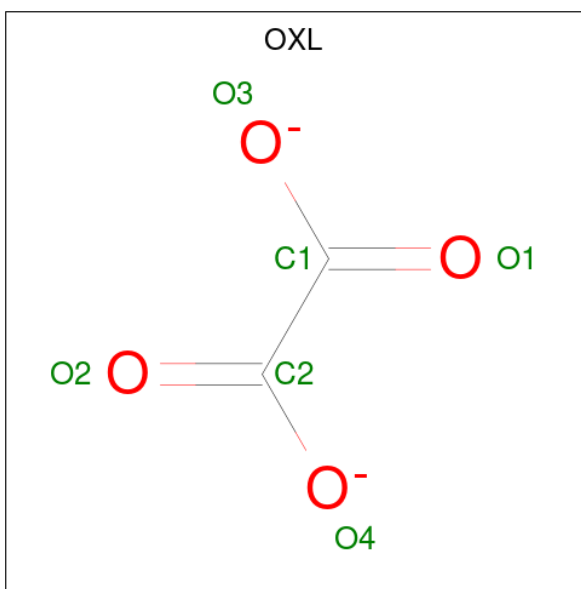
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	GLY	-	expression tag	UNP P14618
B	-16	SER	-	expression tag	UNP P14618
B	-15	SER	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	UNP P14618
B	-12	HIS	-	expression tag	UNP P14618
B	-11	HIS	-	expression tag	UNP P14618
B	-10	HIS	-	expression tag	UNP P14618
B	-9	HIS	-	expression tag	UNP P14618
B	-8	SER	-	expression tag	UNP P14618
B	-7	SER	-	expression tag	UNP P14618
B	-6	GLY	-	expression tag	UNP P14618
B	-5	LEU	-	expression tag	UNP P14618
B	-4	VAL	-	expression tag	UNP P14618
B	-3	PRO	-	expression tag	UNP P14618
B	-2	ARG	-	expression tag	UNP P14618
B	-1	GLY	-	expression tag	UNP P14618
B	0	SER	-	expression tag	UNP P14618
B	70	ASP	ASN	engineered mutation	UNP P14618
C	-18	MET	-	initiating methionine	UNP P14618
C	-17	GLY	-	expression tag	UNP P14618
C	-16	SER	-	expression tag	UNP P14618
C	-15	SER	-	expression tag	UNP P14618
C	-14	HIS	-	expression tag	UNP P14618
C	-13	HIS	-	expression tag	UNP P14618
C	-12	HIS	-	expression tag	UNP P14618
C	-11	HIS	-	expression tag	UNP P14618
C	-10	HIS	-	expression tag	UNP P14618
C	-9	HIS	-	expression tag	UNP P14618
C	-8	SER	-	expression tag	UNP P14618
C	-7	SER	-	expression tag	UNP P14618
C	-6	GLY	-	expression tag	UNP P14618
C	-5	LEU	-	expression tag	UNP P14618
C	-4	VAL	-	expression tag	UNP P14618
C	-3	PRO	-	expression tag	UNP P14618
C	-2	ARG	-	expression tag	UNP P14618
C	-1	GLY	-	expression tag	UNP P14618
C	0	SER	-	expression tag	UNP P14618
C	70	ASP	ASN	engineered mutation	UNP P14618
D	-18	MET	-	initiating methionine	UNP P14618
D	-17	GLY	-	expression tag	UNP P14618
D	-16	SER	-	expression tag	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	SER	-	expression tag	UNP P14618
D	-14	HIS	-	expression tag	UNP P14618
D	-13	HIS	-	expression tag	UNP P14618
D	-12	HIS	-	expression tag	UNP P14618
D	-11	HIS	-	expression tag	UNP P14618
D	-10	HIS	-	expression tag	UNP P14618
D	-9	HIS	-	expression tag	UNP P14618
D	-8	SER	-	expression tag	UNP P14618
D	-7	SER	-	expression tag	UNP P14618
D	-6	GLY	-	expression tag	UNP P14618
D	-5	LEU	-	expression tag	UNP P14618
D	-4	VAL	-	expression tag	UNP P14618
D	-3	PRO	-	expression tag	UNP P14618
D	-2	ARG	-	expression tag	UNP P14618
D	-1	GLY	-	expression tag	UNP P14618
D	0	SER	-	expression tag	UNP P14618
D	70	ASP	ASN	engineered mutation	UNP P14618

- Molecule 2 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).

OXL

O3

O⁻

C1   O   O1

O2   O   C2

O⁻

O4

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 2	O 4	0	0
2	B	1	Total 6	C 2	O 4	0	0
2	C	1	Total 6	C 2	O 4	0	0

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total 6	C 2	O 4	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0
3	B	1	Total 1	Mg 1	0	0
3	C	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
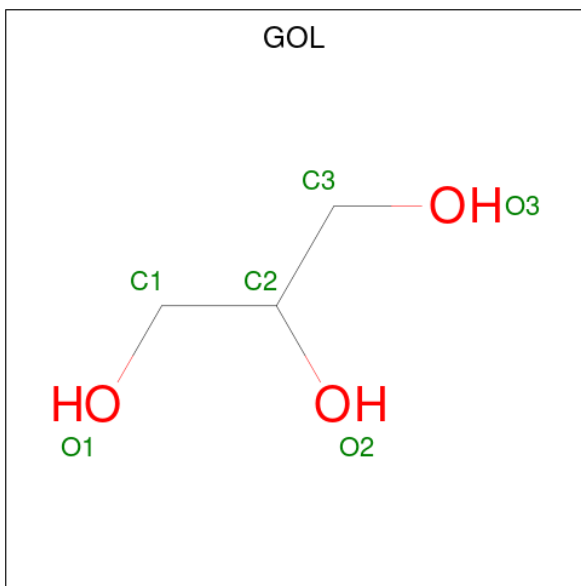
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 6	C 3	O 3		0	0
4	C	1	Total 6	C 3	O 3		0	0
4	C	1	Total 6	C 3	O 3		0	0
4	C	1	Total 6	C 3	O 3		0	0
4	D	1	Total 6	C 3	O 3		0	0
4	D	1	Total 6	C 3	O 3		0	0
4	D	1	Total 6	C 3	O 3		0	0

- Molecule 5 is 1,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: FBP) (formula: $C_6H_{14}O_{12}P_2$).
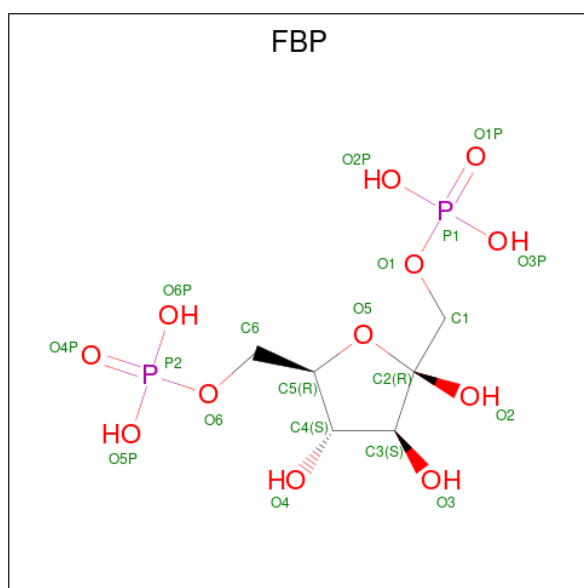
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 8	C 2	O 5	P 1	0	0
5	B	1	Total 5	O 4	P 1		0	0
5	C	1	Total 5	O 4	P 1		0	0
5	D	1	Total 7	C 2	O 4	P 1	0	0

- Molecule 6 is water.

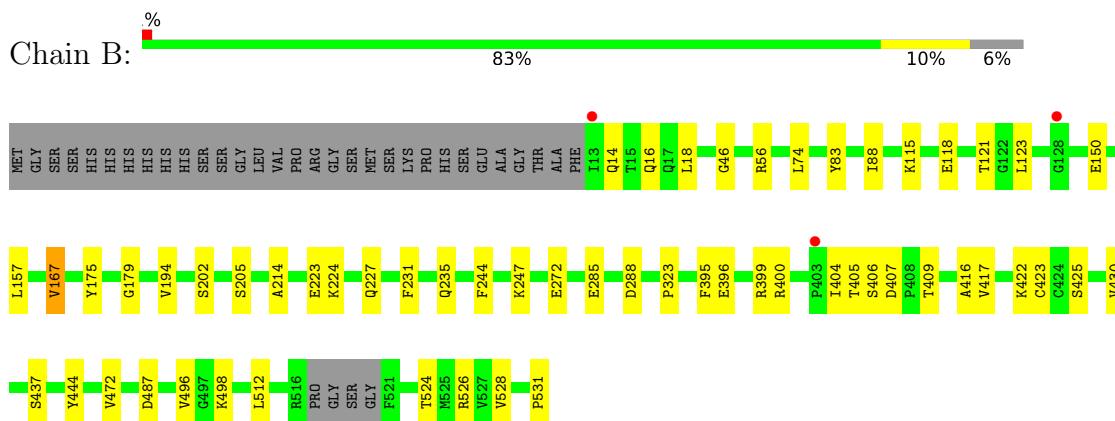| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	191	Total 191	O 191	0	0
6	B	183	Total 183	O 183	0	0
6	C	161	Total 161	O 161	0	0
6	D	129	Total 129	O 129	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
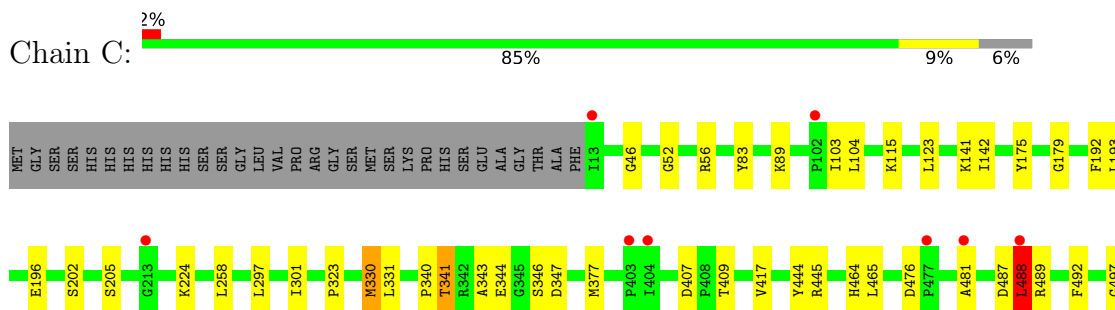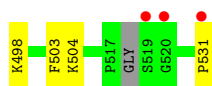
- Molecule 1: Pyruvate kinase PKM

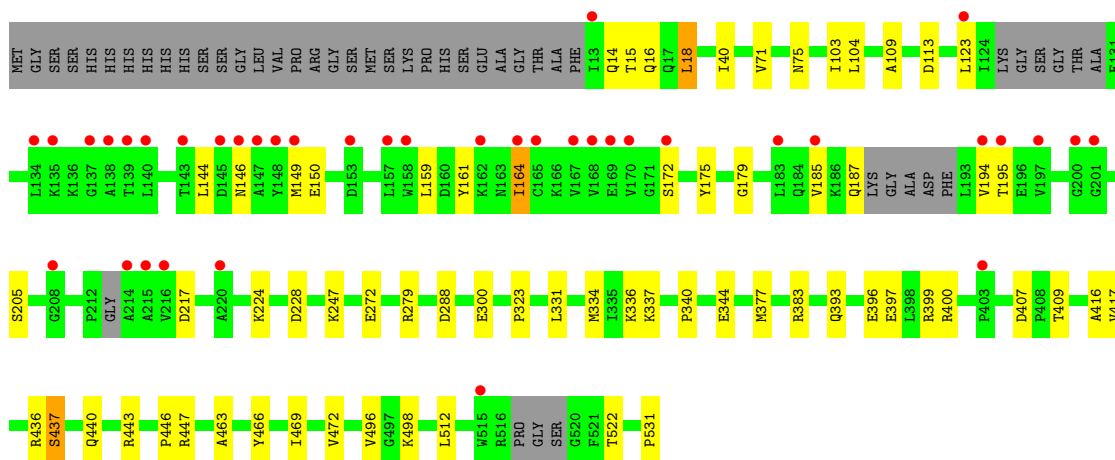Chain A:

- Molecule 1: Pyruvate kinase PKM

Chain B:

- Molecule 1: Pyruvate kinase PKM

Chain C:

K498 F503 K504 P517 GLY S519 G520 P531

• Molecule 1: Pyruvate kinase PKM

Chain D:

7%

79%

12% · 8%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER MET SER LYS PRO HIS SER GLU ALA GLY THR ALA PHE I13 Q14 T15 Q16 Q17 L18 I40 V71 N75 I103 L104 A109 D113 L123 I124 LYS GLY SER GLY THR ALA E131

L134 K135 K136 G137 A138 T139 L140 T143 L144 D145 N146 A147 Y148 M149 E150 D153 L157 W158 L159 D160 Y161 K162 N163 I164 C165 K166 V167 V168 E169 V170 G171 S172 Y175 G179 L183 Q184 V185 K186 Q187 LYS GLY ALA ASP PHE L193 V194 T195 E196 V197 G200 G201

S205 G208 P212 GLY A214 A215 V216 D217 A220 K224 D228 K247 E272 R279 D288 E300 P323 L331 M334 I335 K336 K337 P340 E344 M377 R383 Q393 E396 E397 L398 R399 R400 P403 D407 P408 T409 A416 V417

R436 S437 Q440 R443 P446 R447 A463 Y466 I469 V472 V496 G497 K498 L512 W515 R516 PRO GLY SER G520 F521 T522 P531

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	139.34Å 158.30Å 241.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.81 – 2.29 63.81 – 2.29	Depositor EDS
% Data completeness (in resolution range)	100.0 (63.81-2.29) 100.0 (63.81-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	4.18 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.183 , 0.229 0.183 , 0.228	Depositor DCC
R_{free} test set	5906 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	24.7	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.0	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16070	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FBP, GOL, OXL, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.41	0/3935	0.59	3/5320 (0.1%)
1	B	0.41	0/3921	0.57	0/5308
1	C	0.40	0/3944	0.58	3/5335 (0.1%)
1	D	0.37	0/3714	0.54	0/5034
All	All	0.40	0/15514	0.57	6/20997 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	488	LEU	CA-CB-CG	6.99	131.38	115.30
1	A	516	ARG	N-CA-C	-6.32	93.93	111.00
1	C	488	LEU	CB-CA-C	-6.12	98.57	110.20
1	A	515	TRP	O-C-N	-5.19	114.39	122.70
1	C	488	LEU	CB-CG-CD2	5.17	119.78	111.00
1	A	447	ARG	NE-CZ-NH2	-5.13	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3878	0	3888	22	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3862	0	3867	31	2
1	C	3886	0	3898	28	0
1	D	3661	0	3503	42	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	12	0	16	1	0
4	B	18	0	24	6	0
4	C	18	0	24	3	0
4	D	18	0	24	0	0
5	A	8	0	2	0	0
5	B	5	0	0	1	0
5	C	5	0	0	0	0
5	D	7	0	2	1	0
6	A	191	0	0	2	0
6	B	183	0	0	2	0
6	C	161	0	0	0	0
6	D	129	0	0	2	0
All	All	16070	0	15248	124	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (124) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:488:LEU:O	1:C:488:LEU:HD22	1.53	1.06
1:C:488:LEU:O	1:C:488:LEU:CD2	2.21	0.89
1:C:341:THR:HG22	1:C:344:GLU:H	1.40	0.84
1:B:285:GLU:OE2	6:B:701:HOH:O	2.01	0.79
1:D:144:LEU:HD11	1:D:164:ILE:HD11	1.65	0.79
1:D:185:VAL:HA	1:D:195:THR:HG22	1.64	0.78
1:D:123:LEU:HB2	1:D:150:GLU:HA	1.69	0.74
1:A:183:LEU:HD13	1:A:195:THR:HG21	1.70	0.72
4:B:605:GOL:HO1	4:B:605:GOL:HO3	1.39	0.70
1:D:14:GLN:OE1	6:D:701:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:LYS:NZ	1:C:531:PRO:O	2.30	0.64
1:A:183:LEU:HB3	1:A:195:THR:HG23	1.80	0.63
1:D:123:LEU:HA	1:D:205:SER:HB2	1.79	0.63
1:D:399:ARG:NH2	6:D:704:HOH:O	2.34	0.59
1:B:167:VAL:HG13	1:B:214:ALA:HB1	1.85	0.59
1:B:123:LEU:HD23	1:B:205:SER:HB3	1.84	0.59
1:C:142:ILE:HB	1:C:193:LEU:HB3	1.86	0.58
1:D:498:LYS:NZ	1:D:531:PRO:O	2.31	0.58
1:A:516:ARG:O	1:A:517:PRO:C	2.41	0.57
1:D:103:ILE:HG22	1:D:104:LEU:HD22	1.85	0.57
1:C:487:ASP:O	1:C:488:LEU:HB3	2.05	0.56
1:D:247:LYS:HB3	1:D:279:ARG:HE	1.69	0.56
1:B:498:LYS:NZ	1:B:531:PRO:O	2.38	0.56
1:D:437:SER:OG	5:D:606:FBP:O5P	2.23	0.56
1:B:405:THR:OG1	1:B:406:SER:N	2.38	0.55
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.89	0.55
1:D:159:LEU:HD11	1:D:164:ILE:HD13	1.88	0.55
1:B:244:PHE:HZ	4:B:603:GOL:H31	1.71	0.54
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.42	0.54
1:D:161:TYR:O	1:D:164:ILE:HG12	2.06	0.54
1:C:46:GLY:HA2	4:C:603:GOL:H2	1.89	0.54
1:D:224:LYS:NZ	1:D:228:ASP:OD2	2.37	0.53
1:D:14:GLN:HG3	1:D:15:THR:H	1.72	0.53
1:A:121:THR:HB	1:A:157:LEU:HD11	1.91	0.52
1:D:417:VAL:HG13	1:D:446:PRO:HB3	1.91	0.52
1:D:14:GLN:HG2	1:D:18:LEU:HB2	1.92	0.52
1:D:175:TYR:HB3	1:D:179:GLY:HA2	1.92	0.51
1:B:472:VAL:HG11	1:B:496:VAL:HG11	1.91	0.51
1:C:341:THR:HG23	1:C:343:ALA:H	1.74	0.51
1:A:14:GLN:HB3	6:A:839:HOH:O	2.10	0.51
1:D:340:PRO:HG3	1:D:377:MET:HG2	1.92	0.51
1:C:330:MET:HB3	1:C:347:ASP:OD2	2.11	0.50
1:B:56:ARG:HD2	1:B:83:TYR:OH	2.10	0.50
1:B:396:GLU:O	1:B:400:ARG:HG3	2.11	0.50
1:D:472:VAL:HG11	1:D:496:VAL:HG11	1.93	0.50
1:B:118:GLU:HG2	4:B:603:GOL:H2	1.93	0.50
1:B:526:ARG:HB3	1:B:528:VAL:HG13	1.93	0.50
1:B:175:TYR:HB3	1:B:179:GLY:HA2	1.92	0.50
1:A:123:LEU:HD12	1:A:150:GLU:HG2	1.94	0.49
1:B:115:LYS:NZ	6:B:708:HOH:O	2.44	0.49
1:C:52:GLY:O	1:C:56:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:TYR:CE1	1:A:156:ILE:HD13	2.48	0.49
1:B:437:SER:OG	5:B:606:FBP:O4P	2.25	0.48
1:A:463:ALA:HB1	1:A:469:ILE:HG21	1.95	0.48
1:C:464:HIS:ND1	4:C:603:GOL:O2	2.37	0.48
1:C:46:GLY:CA	4:C:603:GOL:H2	2.43	0.48
1:D:407:ASP:OD2	1:D:436:ARG:NH2	2.46	0.48
1:D:40:ILE:O	1:D:383:ARG:HD2	2.13	0.48
1:A:296:ASP:OD1	4:A:603:GOL:H31	2.14	0.47
1:D:161:TYR:CD2	1:D:164:ILE:HG23	2.49	0.47
1:B:16:GLN:HG3	1:B:18:LEU:HG	1.96	0.47
1:A:183:LEU:HB3	1:A:195:THR:CG2	2.44	0.47
1:C:123:LEU:HD23	1:C:205:SER:HB3	1.96	0.47
1:A:187:GLN:HG3	1:A:194:VAL:HB	1.97	0.47
1:B:223:GLU:O	1:B:227:GLN:HG2	2.15	0.46
1:D:409:THR:HG23	1:D:522:THR:HB	1.97	0.46
1:D:16:GLN:OE1	1:D:447:ARG:HD2	2.15	0.46
1:B:231:PHE:CE2	1:B:235:GLN:HG3	2.51	0.46
1:D:334:MET:HA	1:D:337:LYS:O	2.15	0.46
1:A:16:GLN:HG3	1:A:18:LEU:HG	1.97	0.45
1:D:466:TYR:HB2	1:D:469:ILE:HD12	1.97	0.45
1:A:165:CYS:SG	6:A:867:HOH:O	2.55	0.45
1:C:56:ARG:HD2	1:C:83:TYR:OH	2.16	0.45
1:A:410:GLU:OE2	1:A:440:GLN:NE2	2.50	0.45
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.52	0.45
1:D:159:LEU:HD12	1:D:161:TYR:H	1.80	0.45
1:B:244:PHE:CZ	4:B:603:GOL:H31	2.51	0.45
1:D:463:ALA:HB1	1:D:469:ILE:HG21	1.99	0.45
1:D:161:TYR:OH	1:D:217:ASP:OD2	2.29	0.44
1:A:175:TYR:HB3	1:A:179:GLY:HA2	1.98	0.44
1:A:340:PRO:HG3	1:A:377:MET:HG2	1.98	0.44
1:B:121:THR:HB	1:B:157:LEU:HD11	1.99	0.44
1:A:140:LEU:O	1:A:195:THR:HB	2.18	0.44
1:D:336:LYS:HA	1:D:336:LYS:HD2	1.74	0.44
1:B:423:CYS:SG	1:B:425:SER:HB3	2.58	0.44
1:C:330:MET:O	1:C:331:LEU:HD23	2.17	0.44
1:B:405:THR:HB	1:B:407:ASP:H	1.83	0.43
1:C:407:ASP:OD1	1:C:409:THR:OG1	2.32	0.43
1:D:187:GLN:CB	1:D:194:VAL:H	2.31	0.43
1:B:115:LYS:HD3	1:B:224:LYS:HE3	2.00	0.43
1:C:417:VAL:HG21	1:C:444:TYR:HB2	2.01	0.43
1:D:146:ASN:O	1:D:149:MET:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:LYS:HE2	1:C:192:PHE:CB	2.48	0.43
1:B:288:ASP:O	1:B:323:PRO:HD2	2.19	0.43
1:A:370:TYR:HB3	1:A:373:GLU:HB2	2.01	0.43
1:B:46:GLY:HA2	4:B:604:GOL:H2	2.01	0.43
1:D:18:LEU:HD12	1:D:18:LEU:HA	1.89	0.43
1:D:272:GLU:O	1:D:300:GLU:HG3	2.19	0.43
1:A:456:ASN:HB3	1:A:459:THR:HB	2.01	0.42
1:B:46:GLY:CA	4:B:604:GOL:H2	2.48	0.42
1:B:123:LEU:HD12	1:B:150:GLU:HG2	2.00	0.42
1:B:404:ILE:HD13	1:B:404:ILE:HA	1.84	0.42
1:D:71:VAL:HG22	1:D:109:ALA:HB3	2.01	0.42
1:B:395:PHE:O	1:B:399:ARG:HG3	2.20	0.42
1:C:340:PRO:HG3	1:C:377:MET:HG2	2.01	0.42
1:C:445:ARG:HA	1:C:445:ARG:HD3	1.82	0.42
1:D:396:GLU:O	1:D:400:ARG:HG3	2.19	0.42
1:D:416:ALA:HB2	1:D:512:LEU:HD21	2.02	0.42
1:C:487:ASP:C	1:C:489:ARG:H	2.24	0.41
1:A:158:TRP:CH2	1:A:160:ASP:HB3	2.55	0.41
1:C:323:PRO:HB3	1:C:465:LEU:O	2.21	0.41
1:C:104:LEU:HD23	1:C:104:LEU:HA	1.89	0.41
1:D:331:LEU:HD23	1:D:344:GLU:HB3	2.02	0.41
1:B:416:ALA:HB2	1:B:512:LEU:HD11	2.03	0.41
1:D:75:ASN:HA	1:D:113:ASP:HB3	2.02	0.41
1:B:74:LEU:HD21	1:B:88:ILE:HG13	2.02	0.41
1:D:393:GLN:O	1:D:397:GLU:HG3	2.20	0.41
1:B:417:VAL:HG21	1:B:444:TYR:HB2	2.03	0.40
1:C:115:LYS:HD3	1:C:224:LYS:HD2	2.03	0.40
1:D:288:ASP:O	1:D:323:PRO:HD2	2.22	0.40
1:C:103:ILE:HD13	1:C:492:PHE:HE1	1.86	0.40
1:D:440:GLN:O	1:D:443:ARG:HG2	2.20	0.40
1:C:175:TYR:HB3	1:C:179:GLY:HA2	2.04	0.40
1:C:297:LEU:O	1:C:301:ILE:HG12	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:ILE:CB	1:B:422:LYS:O[3_654]	1.89	0.31
1:A:404:ILE:CA	1:B:422:LYS:O[3_654]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	507/550 (92%)	493 (97%)	14 (3%)	0	100	100
1	B	511/550 (93%)	496 (97%)	15 (3%)	0	100	100
1	C	514/550 (94%)	501 (98%)	12 (2%)	1 (0%)	47	58
1	D	494/550 (90%)	480 (97%)	14 (3%)	0	100	100
All	All	2026/2200 (92%)	1970 (97%)	55 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	481	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/452 (89%)	394 (98%)	10 (2%)	47	65
1	B	402/452 (89%)	392 (98%)	10 (2%)	47	65
1	C	403/452 (89%)	393 (98%)	10 (2%)	47	65
1	D	352/452 (78%)	348 (99%)	4 (1%)	73	86
All	All	1561/1808 (86%)	1527 (98%)	34 (2%)	52	69

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	SER
1	A	163	ASN
1	A	193	LEU
1	A	195	THR
1	A	202	SER
1	A	258	LEU
1	A	401	LEU
1	A	405	THR
1	A	424	CYS
1	A	476	ASP
1	B	14	GLN
1	B	167	VAL
1	B	194	VAL
1	B	202	SER
1	B	247	LYS
1	B	272	GLU
1	B	409	THR
1	B	430	VAL
1	B	487	ASP
1	B	524	THR
1	C	89	LYS
1	C	196	GLU
1	C	202	SER
1	C	258	LEU
1	C	330	MET
1	C	341	THR
1	C	346	SER
1	C	476	ASP
1	C	488	LEU
1	C	504	LYS
1	D	18	LEU
1	D	164	ILE
1	D	172	SER
1	D	437	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	199	ASN
1	D	14	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 4 are monoatomic - leaving 19 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	FBP	D	606	-	6,6,20	1.02	0	8,8,32	0.80	0
4	GOL	B	603	-	5,5,5	0.52	0	5,5,5	1.43	1 (20%)
4	GOL	D	603	-	5,5,5	0.96	0	5,5,5	1.03	0
5	FBP	A	605	-	7,7,20	1.70	2 (28%)	9,9,32	0.86	1 (11%)
4	GOL	C	603	-	5,5,5	1.10	0	5,5,5	0.94	0
4	GOL	B	604	-	5,5,5	0.39	0	5,5,5	1.19	0
2	OXL	B	601	3	5,5,5	1.33	0	6,6,6	1.96	4 (66%)
2	OXL	C	601	3	5,5,5	1.32	0	6,6,6	2.21	4 (66%)
2	OXL	D	601	3	5,5,5	1.19	0	6,6,6	1.88	3 (50%)
4	GOL	D	604	-	5,5,5	0.78	0	5,5,5	1.09	0
5	FBP	B	606	-	4,4,20	2.00	1 (25%)	6,6,32	0.41	0
4	GOL	A	604	-	5,5,5	1.14	1 (20%)	5,5,5	1.01	0
4	GOL	A	603	-	5,5,5	0.64	0	5,5,5	1.08	0
4	GOL	C	605	-	5,5,5	0.87	0	5,5,5	1.12	0
4	GOL	B	605	-	5,5,5	0.79	0	5,5,5	1.27	1 (20%)
2	OXL	A	601	3	5,5,5	1.26	0	6,6,6	2.01	4 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	GOL	C	604	-	5,5,5	1.23	0	5,5,5	0.74	0
4	GOL	D	605	-	5,5,5	0.92	0	5,5,5	0.97	0
5	FBP	C	606	-	4,4,20	3.22	1 (25%)	6,6,32	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	604	-	-	4/4/4/4	-
4	GOL	B	604	-	-	3/4/4/4	-
5	FBP	D	606	-	-	2/4/4/32	-
4	GOL	D	605	-	-	2/4/4/4	-
4	GOL	B	603	-	-	1/4/4/4	-
2	OXL	B	601	3	-	3/4/4/4	-
4	GOL	A	603	-	-	3/4/4/4	-
2	OXL	C	601	3	-	0/4/4/4	-
4	GOL	C	603	-	-	4/4/4/4	-
4	GOL	D	603	-	-	2/4/4/4	-
2	OXL	D	601	3	-	4/4/4/4	-
4	GOL	D	604	-	-	4/4/4/4	-
5	FBP	A	605	-	-	1/5/5/32	-
4	GOL	C	605	-	-	2/4/4/4	-
4	GOL	B	605	-	-	0/4/4/4	-
2	OXL	A	601	3	-	4/4/4/4	-
4	GOL	A	604	-	-	4/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	606	FBP	P2-O4P	6.27	1.65	1.50
5	A	605	FBP	O5-C5	3.84	1.61	1.42
5	B	606	FBP	P2-O6	3.80	1.66	1.54
4	A	604	GOL	C3-C2	2.23	1.60	1.51
5	A	605	FBP	P2-O6	2.13	1.67	1.60

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	OXL	O4-C2-C1	3.24	122.78	113.16
2	A	601	OXL	O4-C2-C1	2.75	121.32	113.16
2	D	601	OXL	O3-C1-C2	2.70	121.19	113.16
2	B	601	OXL	O4-C2-C1	2.67	121.08	113.16
4	B	603	GOL	C3-C2-C1	-2.62	101.50	111.70
2	C	601	OXL	O3-C1-O1	-2.62	117.61	123.61
2	C	601	OXL	O3-C1-C2	2.59	120.86	113.16
2	A	601	OXL	O4-C2-O2	-2.57	117.73	123.61
2	A	601	OXL	O3-C1-O1	-2.41	118.10	123.61
2	D	601	OXL	O4-C2-C1	2.38	120.22	113.16
2	B	601	OXL	O3-C1-C2	2.37	120.20	113.16
2	B	601	OXL	O3-C1-O1	-2.34	118.25	123.61
5	A	605	FBP	O6P-P2-O6	2.28	112.80	106.73
4	B	605	GOL	C3-C2-C1	-2.23	103.04	111.70
2	C	601	OXL	O4-C2-O2	-2.19	118.60	123.61
2	B	601	OXL	O4-C2-O2	-2.16	118.68	123.61
2	D	601	OXL	O3-C1-O1	-2.11	118.79	123.61
2	A	601	OXL	O3-C1-C2	2.00	119.10	113.16

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	OXL	O1-C1-C2-O2
2	D	601	OXL	O1-C1-C2-O4
2	D	601	OXL	O3-C1-C2-O4
4	A	603	GOL	C1-C2-C3-O3
4	B	604	GOL	O1-C1-C2-C3
4	C	603	GOL	O1-C1-C2-O2
4	C	603	GOL	O1-C1-C2-C3
4	C	604	GOL	O1-C1-C2-C3
4	C	604	GOL	C1-C2-C3-O3
4	C	605	GOL	C1-C2-C3-O3
4	C	605	GOL	O2-C2-C3-O3
4	D	604	GOL	O1-C1-C2-C3
4	D	605	GOL	C1-C2-C3-O3
5	D	606	FBP	C6-O6-P2-O5P
5	D	606	FBP	C6-O6-P2-O6P
2	D	601	OXL	O3-C1-C2-O2
4	C	604	GOL	O2-C2-C3-O3
4	D	605	GOL	O2-C2-C3-O3
4	A	604	GOL	O1-C1-C2-C3
4	A	604	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	603	GOL	C1-C2-C3-O3
4	C	603	GOL	C1-C2-C3-O3
4	D	604	GOL	C1-C2-C3-O3
4	A	604	GOL	O1-C1-C2-O2
4	B	604	GOL	O1-C1-C2-O2
4	D	604	GOL	O1-C1-C2-O2
4	D	604	GOL	O2-C2-C3-O3
2	A	601	OXL	O1-C1-C2-O2
4	A	604	GOL	O2-C2-C3-O3
4	C	604	GOL	O1-C1-C2-O2
4	A	603	GOL	O2-C2-C3-O3
4	C	603	GOL	O2-C2-C3-O3
5	A	605	FBP	O5-C5-C6-O6
4	B	604	GOL	C1-C2-C3-O3
2	A	601	OXL	O3-C1-C2-O4
2	A	601	OXL	O1-C1-C2-O4
2	A	601	OXL	O3-C1-C2-O2
4	A	603	GOL	O1-C1-C2-O2
2	B	601	OXL	O1-C1-C2-O2
2	B	601	OXL	O3-C1-C2-O4
4	D	603	GOL	O1-C1-C2-C3
4	D	603	GOL	C1-C2-C3-O3
2	B	601	OXL	O1-C1-C2-O4

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	606	FBP	1	0
4	B	603	GOL	3	0
4	C	603	GOL	3	0
4	B	604	GOL	2	0
5	B	606	FBP	1	0
4	A	603	GOL	1	0
4	B	605	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand FBP D 606

Bond lengths

Bond angles

Torsions

Rings

Ligand FBP A 605

Bond lengths

Bond angles

Torsions

Rings

Ligand FBP B 606

Bond lengths

Bond angles

Torsions

Rings

Ligand FBP C 606

Bond lengths — Bond angles — Torsions — Rings
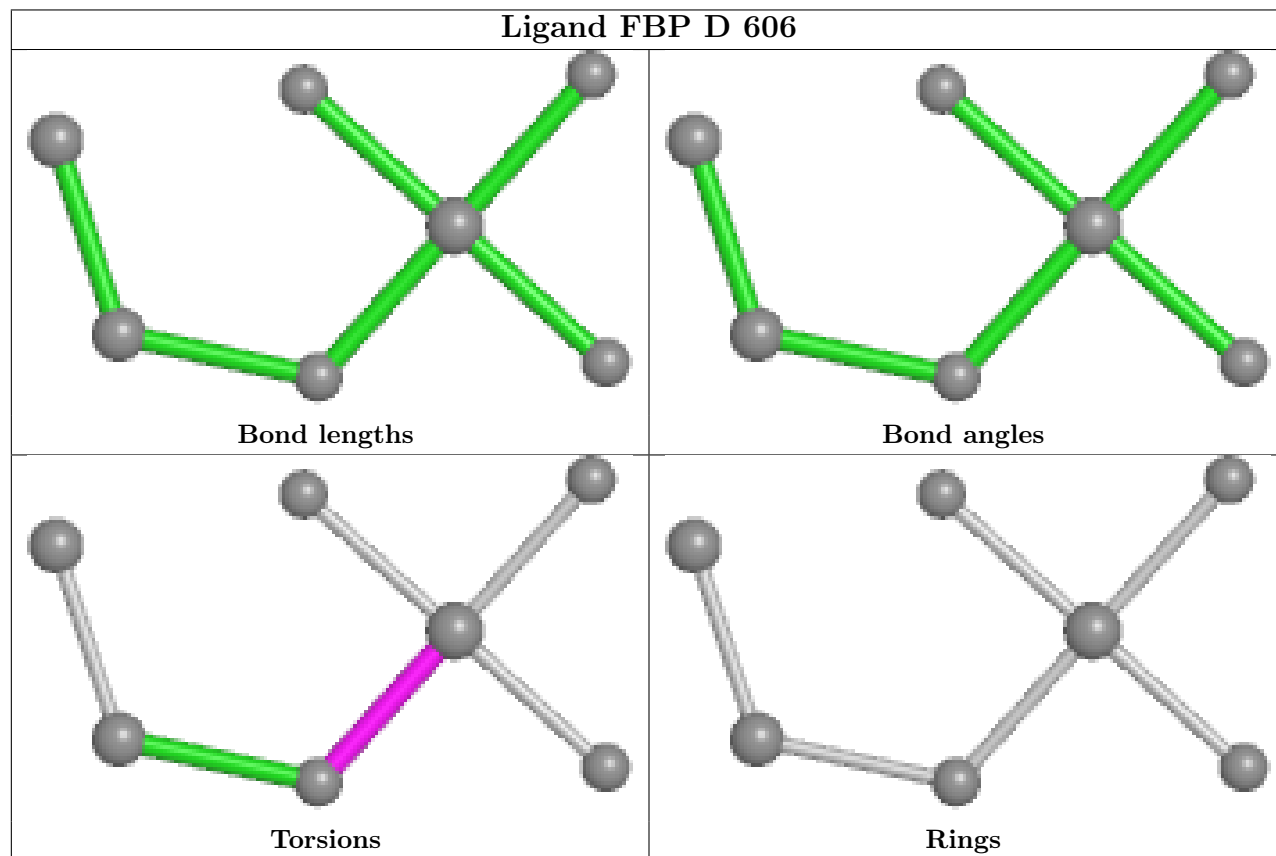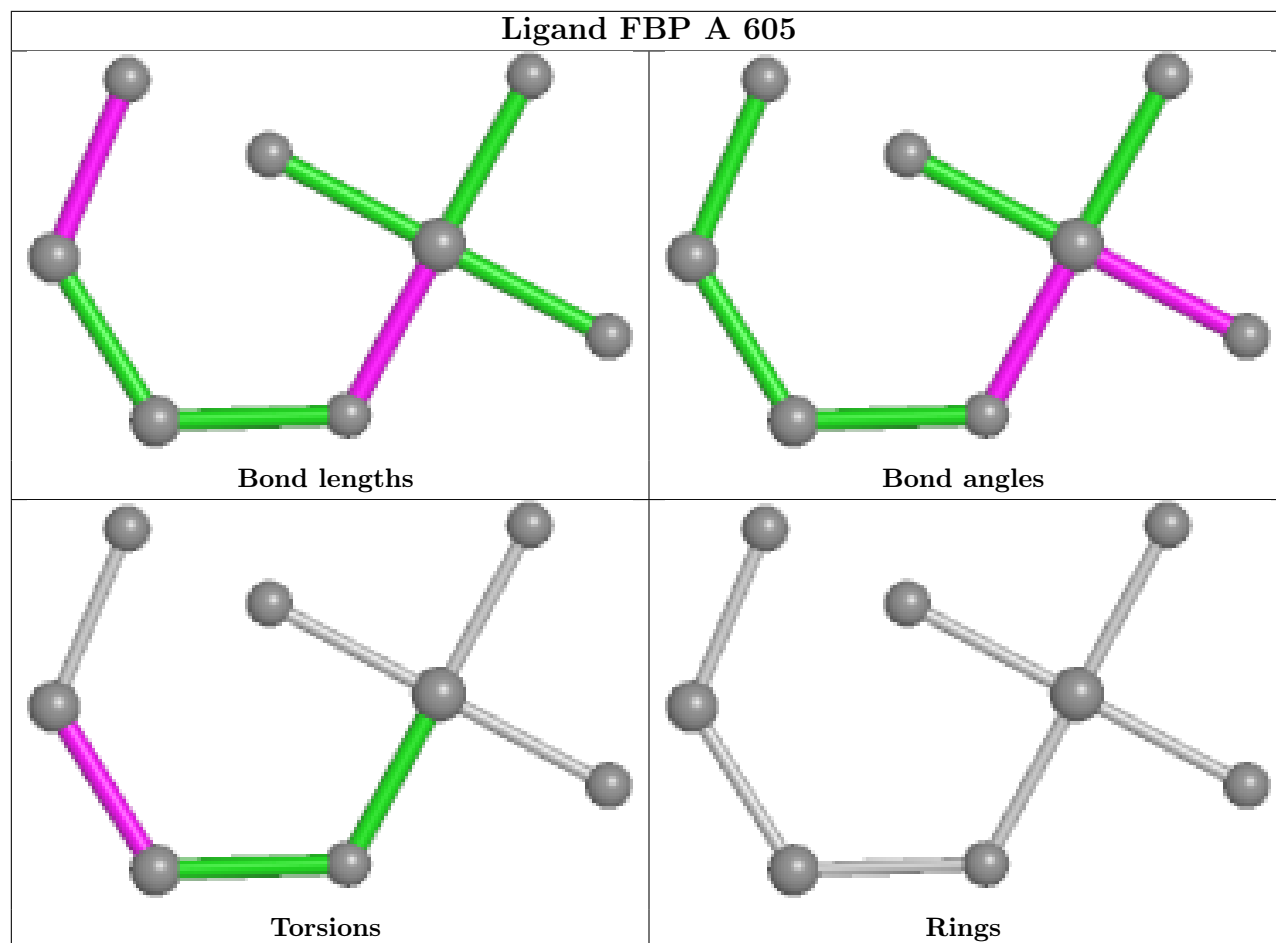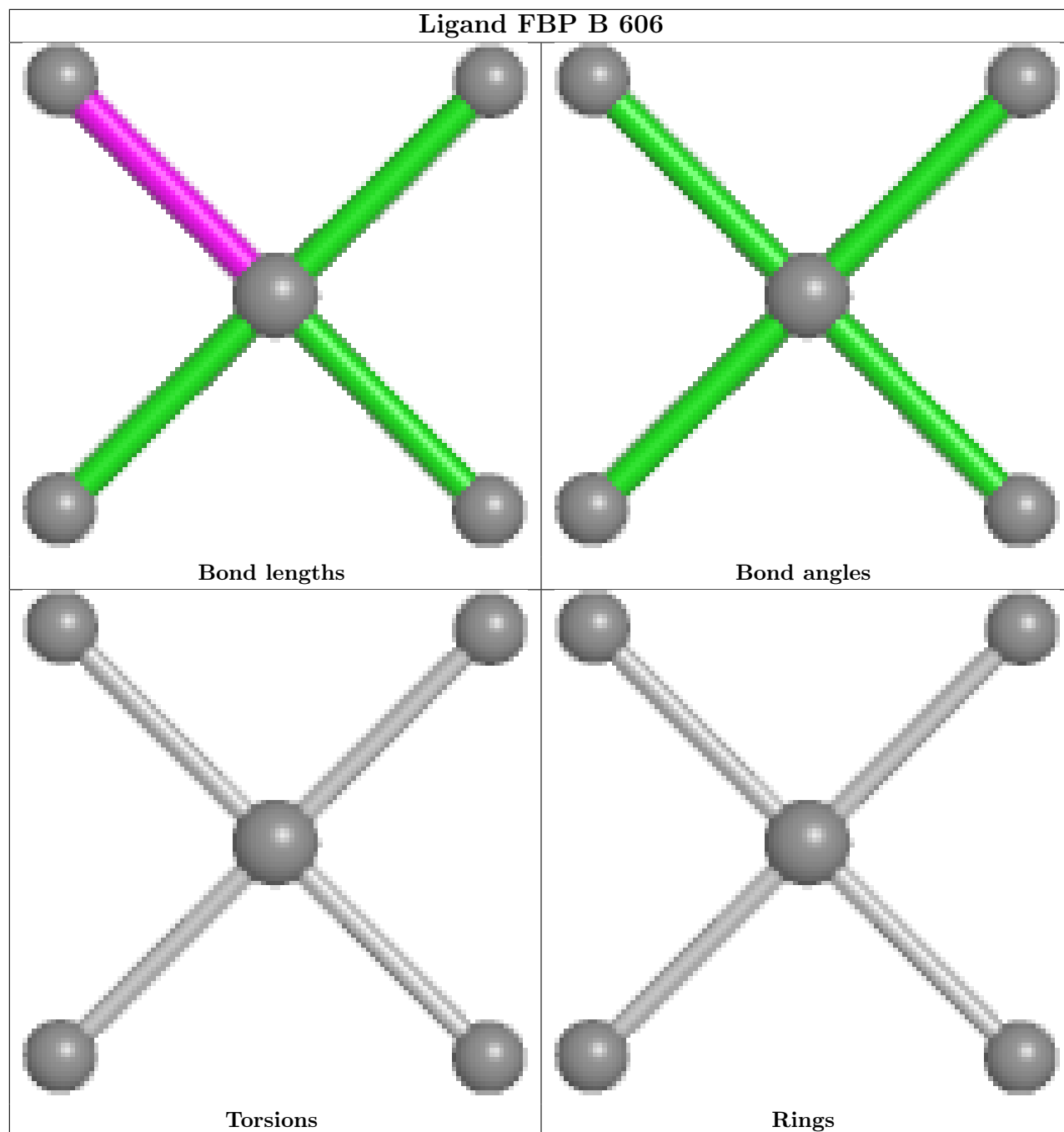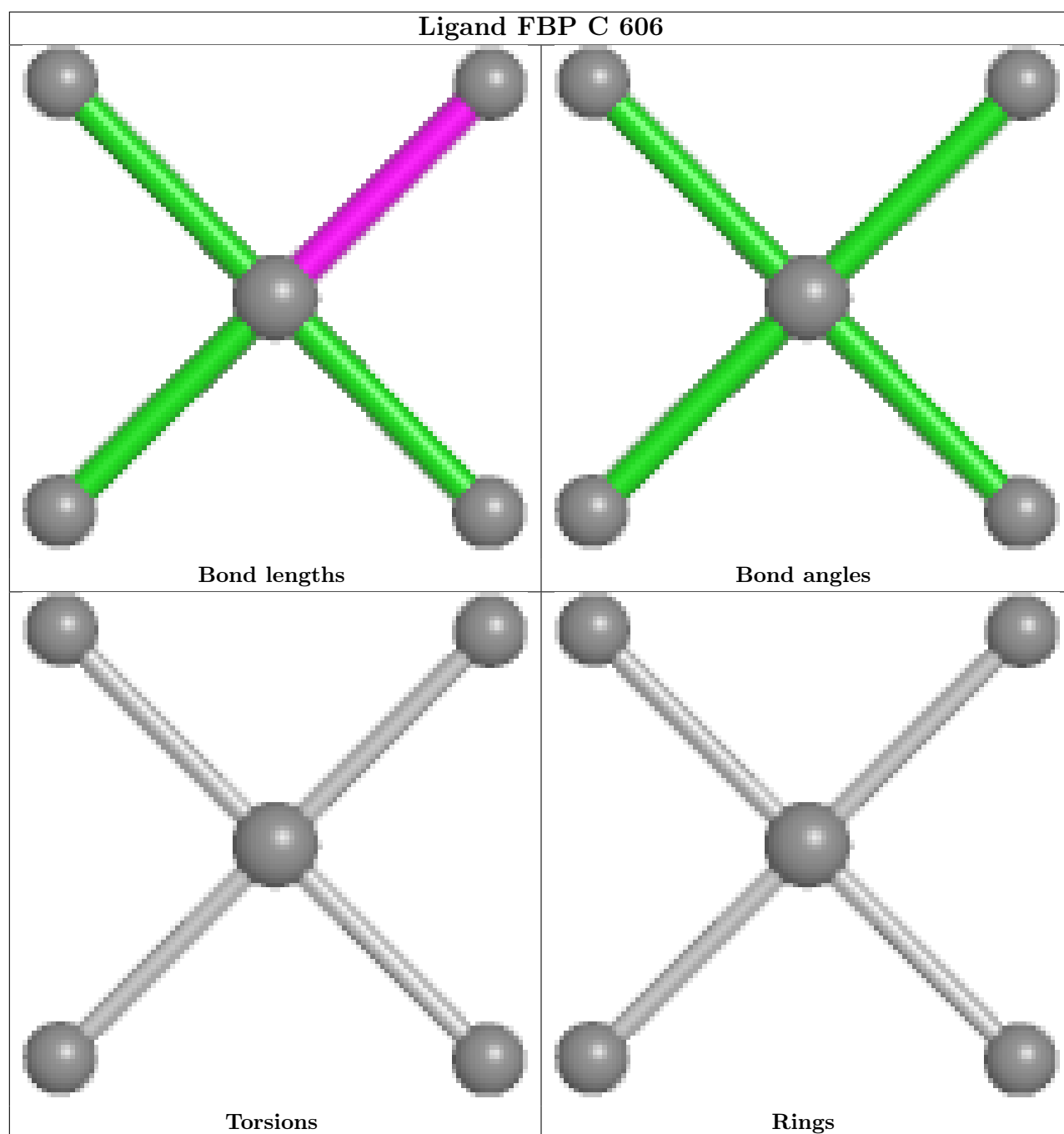
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	515/550 (93%)	-0.24	10 (1%)	66	73	13, 25, 45, 76	0
1	B	515/550 (93%)	-0.28	3 (0%)	89	92	12, 27, 48, 67	0
1	C	518/550 (94%)	-0.21	11 (2%)	63	70	14, 27, 50, 66	0
1	D	504/550 (91%)	0.16	39 (7%)	13	17	14, 32, 70, 89	0
All	All	2052/2200 (93%)	-0.14	63 (3%)	49	56	12, 27, 58, 89	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	404	ILE	8.3
1	B	13	ILE	6.8
1	D	165	CYS	6.3
1	A	403	PRO	6.1
1	D	170	VAL	5.9
1	A	405	THR	5.7
1	D	137	GLY	5.5
1	D	214	ALA	5.3
1	A	13	ILE	5.1
1	A	129	THR	5.0
1	D	515	TRP	4.6
1	C	13	ILE	4.4
1	C	404	ILE	4.3
1	D	195	THR	4.2
1	A	128	GLY	4.1
1	D	13	ILE	3.9
1	D	164	ILE	3.8
1	D	143	THR	3.8
1	B	403	PRO	3.7
1	C	519	SER	3.6
1	D	147	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	169	GLU	3.5
1	A	518	GLY	3.5
1	D	123	LEU	3.4
1	D	140	LEU	3.3
1	D	215	ALA	3.2
1	D	139	THR	3.0
1	C	481	ALA	3.0
1	D	200	GLY	2.9
1	D	172	SER	2.9
1	A	406	SER	2.9
1	D	194	VAL	2.9
1	C	520	GLY	2.9
1	D	183	LEU	2.9
1	D	208	GLY	2.9
1	C	403	PRO	2.8
1	D	216	VAL	2.8
1	D	134	LEU	2.8
1	A	477	PRO	2.7
1	C	488	LEU	2.6
1	D	158	TRP	2.6
1	D	168	VAL	2.6
1	D	197	VAL	2.6
1	C	213	GLY	2.6
1	B	128	GLY	2.5
1	D	153	ASP	2.5
1	D	201	GLY	2.5
1	D	167	VAL	2.4
1	D	162	LYS	2.4
1	D	157	LEU	2.4
1	D	138	ALA	2.4
1	C	531	PRO	2.4
1	D	145	ASP	2.3
1	D	149	MET	2.3
1	D	146	ASN	2.3
1	D	148	TYR	2.3
1	D	185	VAL	2.3
1	D	403	PRO	2.3
1	A	517	PRO	2.2
1	C	102	PRO	2.2
1	D	135	LYS	2.2
1	C	477	PRO	2.1
1	D	220	ALA	2.1

6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
4	GOL	D	603	6/6	0.82	0.21	27,31,35,36	0
4	GOL	B	603	6/6	0.86	0.20	24,29,31,38	0
4	GOL	C	603	6/6	0.88	0.22	27,31,34,34	0
4	GOL	B	604	6/6	0.88	0.20	26,27,30,30	0
4	GOL	D	605	6/6	0.89	0.32	40,40,44,46	0
5	FBP	D	606	7/20	0.89	0.20	33,44,48,51	7
4	GOL	C	604	6/6	0.90	0.19	38,39,43,44	0
4	GOL	A	603	6/6	0.90	0.19	24,28,34,41	0
5	FBP	A	605	8/20	0.91	0.11	27,33,39,43	8
4	GOL	D	604	6/6	0.91	0.15	33,38,40,50	0
4	GOL	A	604	6/6	0.92	0.18	29,31,34,35	0
5	FBP	C	606	5/20	0.93	0.14	32,32,43,44	5
3	MG	D	602	1/1	0.93	0.08	35,35,35,35	0
4	GOL	B	605	6/6	0.94	0.27	35,39,42,42	0
2	OXL	B	601	6/6	0.95	0.10	21,22,30,31	0
3	MG	A	602	1/1	0.95	0.09	23,23,23,23	0
2	OXL	D	601	6/6	0.96	0.10	25,31,35,42	0
4	GOL	C	605	6/6	0.96	0.12	23,34,36,40	0
5	FBP	B	606	5/20	0.97	0.09	24,29,37,41	5
2	OXL	C	601	6/6	0.97	0.11	21,23,29,36	0
2	OXL	A	601	6/6	0.97	0.11	22,24,32,33	0
3	MG	B	602	1/1	0.98	0.04	24,24,24,24	0
3	MG	C	602	1/1	0.98	0.04	19,19,19,19	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FBP D 606:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
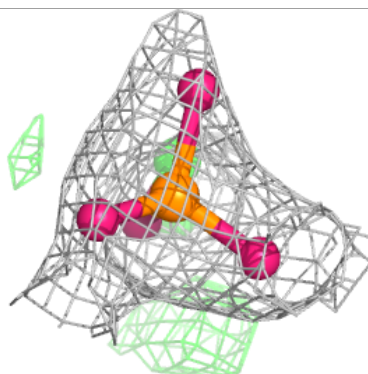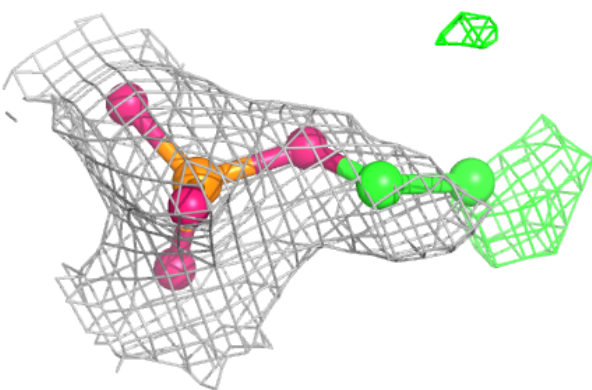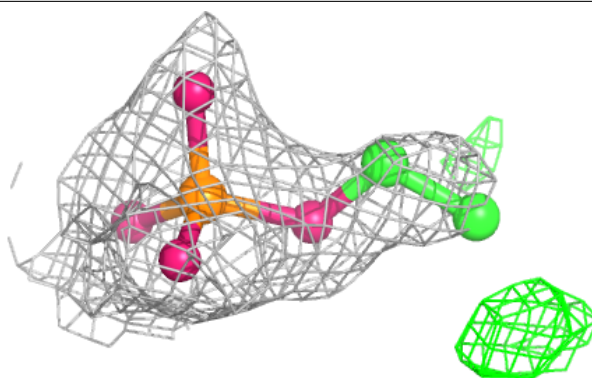
Electron density around FBP A 605:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
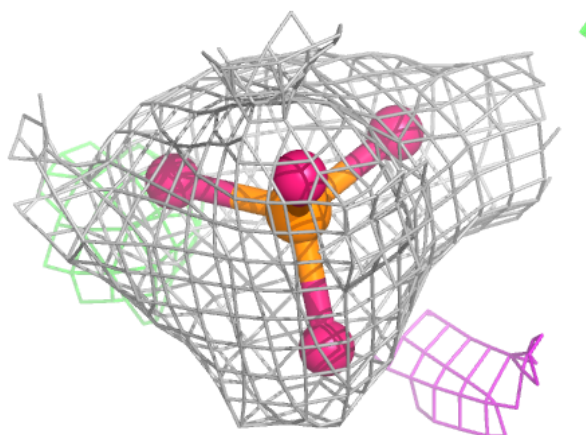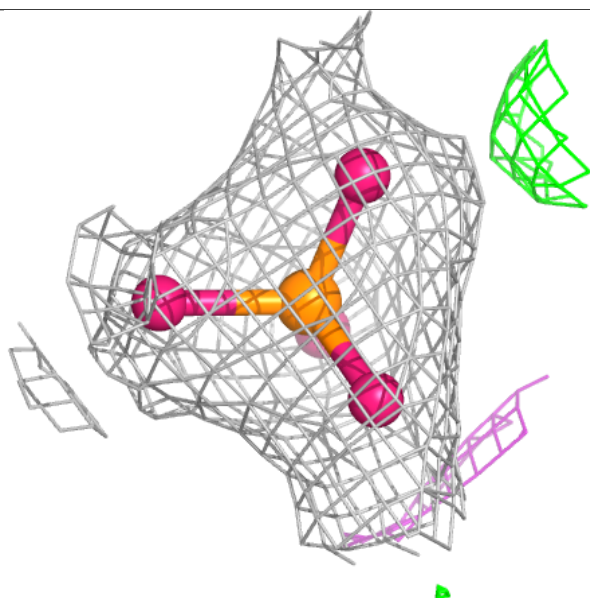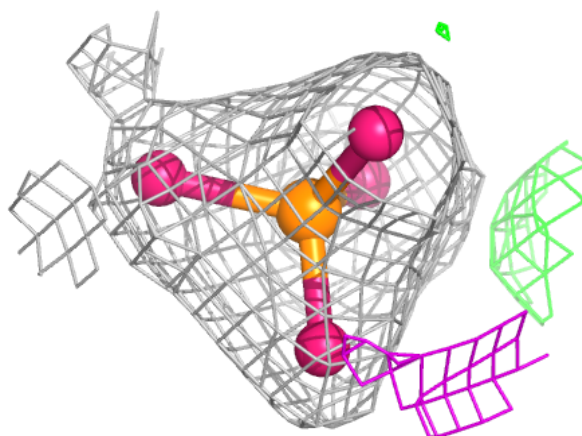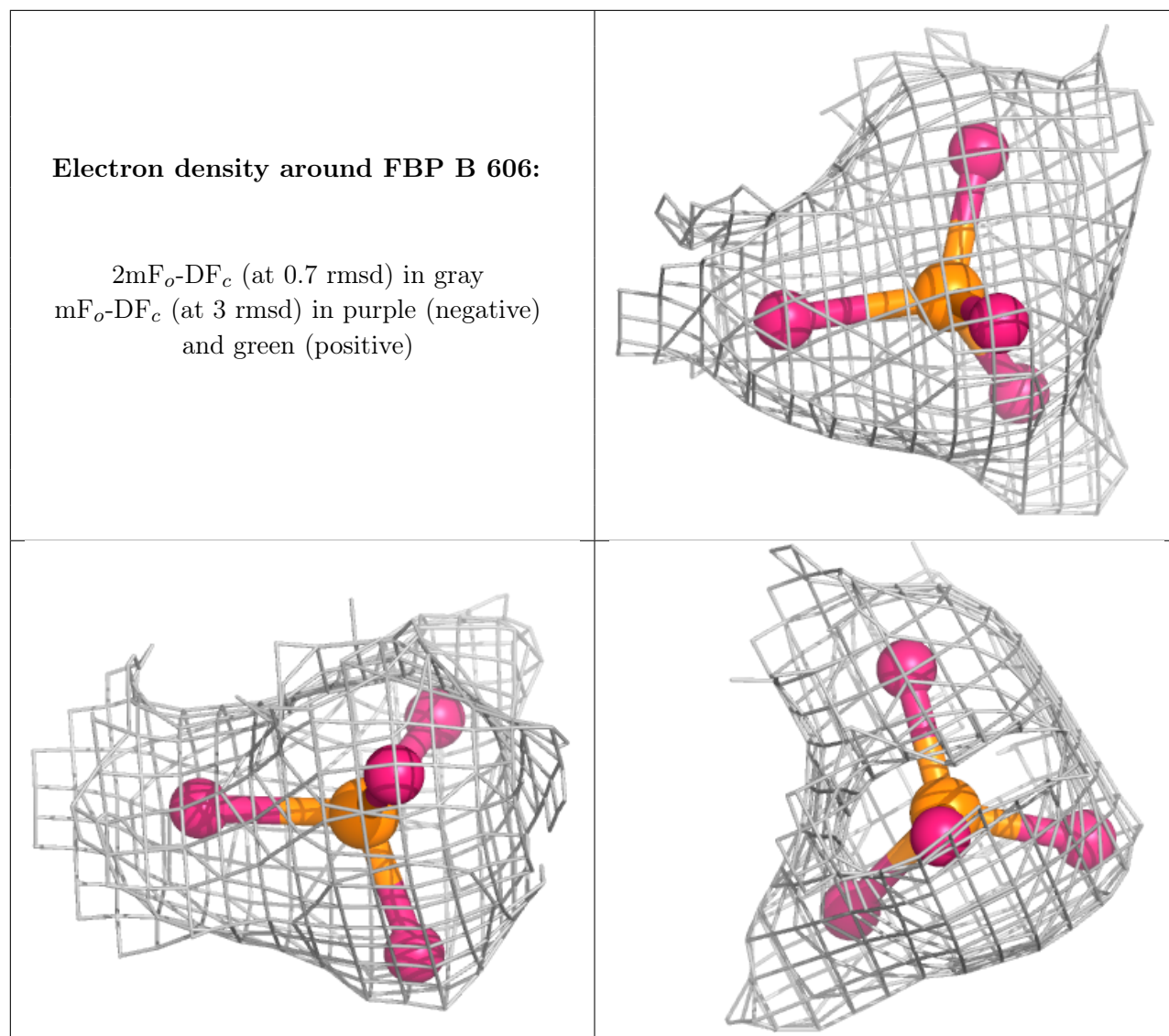mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
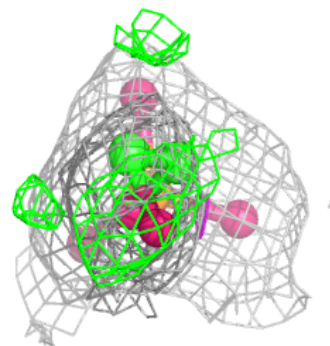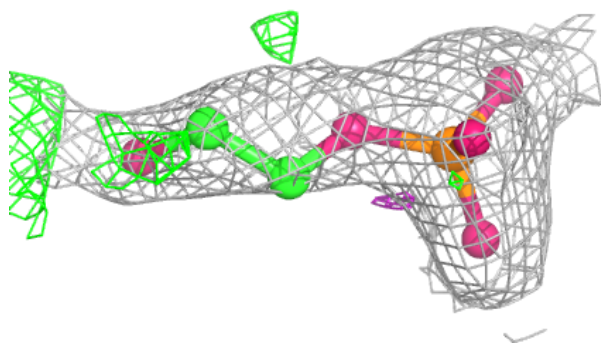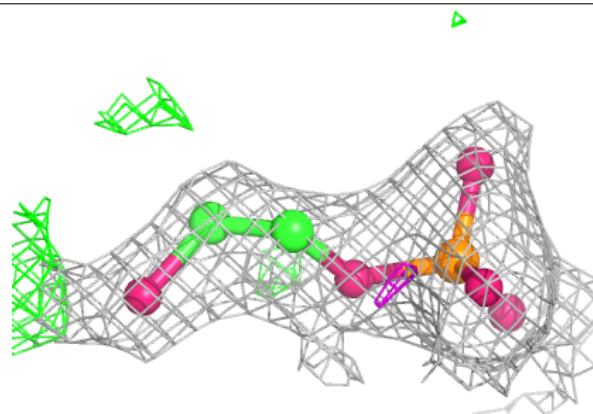
Electron density around FBP C 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around FBP B 606:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers (i)

There are no such residues in this entry.